the longer leg of the bridge is to B_{III} which is bound to two such hydrogen atoms.

The closest approach of hydrogen atoms within the molecule is 1·98 A. The intermolecular contacts are all through hydrogen atoms, and the shortest distances are in the range 2·5–3·0 A.

Chemical implications

In attempting to understand the strange structure of the molecule and the peculiar bonding within it, the most successful interpretation has been in terms of resonating single bonds, such as used by Pauling (1947) in describing metallic binding.

In Fig. 12 there are given (in addition to the bond distances) bond numbers, as defined by Pauling. They have not been derived from the equation of Pauling relating bond number to interatomic distance, but as follows. Each of the regular B–H's is considered to be a full covalent bond and hence of bond number 1. Four boron atoms (B_{II}, B'_{II}, B_V, B'_V) then each have five equivalent bonds to boron, among which two electrons are to be distributed. These bonds are consequently assigned a bond number of 0·4. In order to keep the valence of B_{III} at three, the longer legs of the hydrogen bridges would need to be of bond number 0·4—this in turn makes the bond number for the shorter legs 0·6 and for the long B–B bond 0·2. In other words, with this assignment of bond numbers each boron is trivalent and each hydrogen monovalent. The relation used by Pauling is $R(1) - R(n) = 0{\cdot}3 \log n$, where n is the bond number, and $R(1)$ and $R(n)$ are respectively the radius for a single covalent bond and for one of bond number n. From this relation the value of $R(1)$ is 0·77 A. if calculated from the B–B bonds of 1·77 and 0·80 A. from the long bond of 2·01 A. The value given by Pauling is 0·80 A.

Although this description may not be the best one, it is rather definite that the binding within the molecule is of the 'metallic' type with a mobile system of electrons, and for which the bonds have directional properties different from those ascribed to normal covalent linkages.

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The Probability Distribution of X-ray Intensities. IV. New Methods of Determining Crystal Classes and Space Groups

By D. Rogers

Viriamu Jones Laboratory, University College, Cardiff, Wales

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The application of the two methods of intensity statistics, the 'distribution method' and the 'method of averages', to the identification of the symmetry elements in a crystal is discussed. It is shown that each symmetry element has a distinct and recognizable effect on the weighted reciprocal lattice, and it is concluded that, from X-ray intensities alone, each crystal class may theoretically be identified uniquely. As a result 215 of the 219 space groups are also by these methods uniquely identifiable from X-ray data. Information concerning symmetry elements may also be obtained which is of value in structural investigations. A brief consideration is given to the remaining two pairs of space groups $I222$, $I2_12_12_1$ and $I23$, $I2_13$.

1. Introduction

The recent theoretical work on X-ray intensity statistics (Wilson, 1949, 1950) has shown that, except in certain foreseeable cases, the distribution of the structure amplitudes of the reflexions should conform to one or other of two Gaussian types. When the structure amplitude can be represented by $F \equiv x+iy$, the probability distribution of the F vectors in the complex (x, y) plane has (except for low orders) circular symmetry and a Gaussian variation in the radial direction. This, when integrated over the annuli, gives the function

$$ {}_1P(I) = S^{-1} \exp(-I/S), \qquad (1)$$

as the probability of finding a reflexion of intensity I. The quantity S is the distribution parameter appropriate to the set of reflexions under consideration. Its possible values will be discussed in § 3.

In a set of reflexions whose structure amplitudes are *systematically real* ($F = x+i0$) the vectors are confined to the x axis and again have a Gaussian distribution which leads to the function

$$ {}_{\bar{1}}P(I) = (2\pi SI)^{-\frac{1}{2}} \exp(-I/2S) \qquad (2)$$

as the probability in such a case. This implies a substantially higher proportion of very weak and accidentally absent reflexions, a distinction arising directly from the integration geometry.

Both intensity distributions have been confirmed experimentally by Howells, Phillips & Rogers (1949, 1950), who have shown that the distinction is sufficiently marked to provide a satisfactory and rapid means of discrimination. A statistical survey of the intensities to discriminate between these two distribution functions will be referred to throughout this paper as the *distribution method* and is considered in detail in § 2.

Wilson (1950) has also shown that the average intensities of certain groups of reflexions are small integral multiples of those for the general reflexions. The groups affected and their average multiples, n, are characteristic of the symmetry elements in the space group. Thus a second statistical method is available for the identification of symmetry elements. This, which will be called *the method of averages*, seeks zones or central reciprocal-lattice rows with abnormal intensity averages or distribution parameters. It is discussed fully in § 3.

The object of this paper is to consider the extent to which these two new techniques permit the identification of crystal classes, space groups and those symmetry elements not hitherto identifiable by X-ray means. It will be shown that each symmetry element leaves a characteristic impress on the weighted reciprocal lattice† which can now be readily recognized, a fact which transforms the problem of space-group identification and provides other valuable aids.

Hitherto it has been possible to derive from the systematic properties of the X-ray data only the Laue symmetry of the diffraction effects and evidence for those symmetry elements involving translation, the former from the point-group symmetry of the intensity array and the latter from the systematic absences ($F \equiv 0$) among the reflexions. The remaining symmetry elements were not known to produce other types of systematic peculiarity in the intensity array and could not, therefore, be recognized from X-ray evidence.

A list of 121 diffraction symbols‡ was drawn up by Buerger (1942) to describe each of the patterns identifiable on the basis of Laue symmetry and systematic absences. In this way only forty-nine space groups and the eleven enantiomorphous pairs are determined unambiguously; these are scattered throughout the crystal classes. All the remaining diffraction symbols involve space-group ambiguities.

No X-ray method was hitherto available for the identification of the crystal classes. Tests for pyro- and piezo-electricity are of value only when a positive result is obtained and often even then leave classes unresolved, e.g. 2 and m. Morphological examinations are not always possible and may prove misleading. On the other hand, since such tests can be applied more quickly than those to be discussed in this paper, the new methods should be regarded as supplementary. They are capable of giving unequivocal decisions, subject to certain conditions being fulfilled (Howells *et al.* 1950), but would be used to arbitrate only when the quicker methods fail or yield doubtful results. The ability of Patterson syntheses to discriminate in some suitable problems is recognized. Harker sections and in particular Buerger's implication technique (1946) are also useful, but their value in dealing with typical complex and 'featureless' organic structures remains unproven, whereas the present methods are at their best for just such substances. Moreover, the experimental work and computation for any type of Patterson procedure are much greater than are required for either statistical method.

It will be shown that the new methods provide means for identifying all the crystal classes, and also permit the identification of some symmetry elements of value in structural work which were not previously identifiable. Among the 230 space groups are eleven pairs of enantiomorphs (the members of six pairs being distinguishable but not identifiable by X-ray diffraction procedures (ter Berg & Jaeger, 1937)). Nowacki (1942), therefore, regards the entire list as consisting of 219 space groups; it will be shown that all but four of these are now uniquely identifiable. The four occur in two unresolved pairs, $I222$, $I2_12_12_1$ and $I23$, $I2_13$, discussed in § 4.

2. The distribution method

In addition to those reflexions which are *systematically absent* we can now identify those sets which are *systematically real* and use them for determinative purposes. They will be described briefly as *centric* (Rogers, 1949),

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† The weight assigned to each reciprocal-lattice point may be either the structure amplitude, F, or the intensity, $|F|^2$. These will be termed the *amplitude* (or F) *array* and the *intensity* (or I) *array* respectively; the latter is referred to throughout this paper. The term array has been chosen to avoid the obvious ambiguity in the expression F (or I) lattice.

‡ The number may be increased by two if in Laue symmetry $\bar{3}m$ it is indicated whether the symmetry planes of the intensity array are the zones $[h\bar{h}0l]$ or $[h.h.\overline{2h}.l]$. Thus Buerger's two symbols $\bar{3}mC---$ and $\bar{3}m\mathrm{C}3_1--$ become $\bar{3}m1C---$, $\bar{3}1mC---$ and $\bar{3}m1C3_1--$, $\bar{3}1mC3_1--$.

while sets of reflexions whose structure amplitudes are not systematically real will be termed *acentric*. For clarity and brevity these terms will be used henceforth to describe both the sets of reflexions and their characteristic intensity distributions, while the terms *centrosymmetric* and *non-centrosymmetric* will be reserved for the crystal lattice and its projections.

Structure amplitudes will be systematically real whenever they are associated with a centre of symmetry. This can occur in three ways under conditions listed for each space group in the *Structure Factor Tables* of Lonsdale (1936) or deducible from the *International Tables* (vol. 1):

(1) For a centrosymmetric space group, referred to the symmetry centre as origin, all the F's are real. The entire intensity array (and thus any zone) is therefore centric.

(2) Projections along $2, 4, \bar{4}, 6$ (and their screws) are centrosymmetric even though the space group is not. When the centre of symmetry of the projection is taken as origin all the structure amplitudes in the corresponding *zone* are real. This zone only is therefore centric.

(3) One-dimensional projections will be centrosymmetric if the axis of projection is parallel to $\bar{2}$ $(\equiv m), \bar{4}, \bar{6}$. The corresponding central lattice row is then centric.

The use as origin of any point other than the centre of symmetry cannot affect the distribution of intensities, but will cause the F vectors systematically to occupy certain positions only in the x, y plane; e.g. F is alternately real and imaginary when the origin is midway between symmetry centres (see also theorems (1) and (2), Buerger, 1949).

Table 1 summarizes the centric sets of reflexions produced by each symmetry element. These, taken in conjunction with the known Laue symmetry, provide unique characterization of each symmetry element when it occurs alone.

Table 2 (columns 2, 3) summarizes the characteristic features of each of the thirty-two point groups. The notation is an extension of Buerger's (1942). A centric intensity array (condition 1) is denoted by a bar under the cell-type symbol *only*. A centric zone (condition 2) is indicated by a bar under the appropriate entry in the diffraction symbol. A centric row (condition 3) is indicated by the circumflex (∧) placed over the appropriate entry, but it is recorded only for $\bar{4}$, as it forms the only means, by this method, of distinguishing between 4 and $\bar{4}$. The sets of centric reflexions recorded in column 3 are, however, complete, and it will be noted that centric rows are frequently masked by centric zones. Both the row and zone are then placed within square brackets.

In practice the limited number of reflexions in a row will rarely be sufficient for satisfactory recognition of the type of distribution. Fortunately, however, the method of averages offers a more satisfactory means of identifying $\bar{2}$, $\bar{4}$ and $\bar{6}$, so that it will be very rarely necessary to apply the distribution method to a single reciprocal-lattice row.

It is concluded from Table 2 that, with the possible exception of 4 and $\bar{4}$, each crystal class may now be identified uniquely from X-ray intensity data by an application of the distribution method.

A very useful table for the determination of space groups may be constructed† by adding the above signs to the entries in Buerger's (1942) table of diffraction symbols.

We may consider as an example the Buerger diffraction symbol $6/mmmC-/---$ given by the five space groups which, with their new diffraction symbols, are:

(*a*) $6/mmmC-/--\underline{-}$ $\equiv C\bar{6}m2$,
(*b*) $6/mmmC-/-\underline{-}-$ $\equiv C\bar{6}2m$,
(*c*) $6/mmmC-/\underline{-}--$ $\equiv C6mm$,
(*d*) $6/mmmC-/\underline{-}\,\underline{-}\,\underline{-}$ $\equiv C62$,
(*e*) $6/mmm\underline{C}-/---$ $\equiv C6/mmm$.

These are interpreted as follows:

(1) Laue symmetry $6/mmm$.
(2) Primitive hexagonal (C) lattice.
(3) No systematic absences.
(4) Only $\{hh\overline{2h}l\}$ reflexions centric in (*a*).
Only $\{h0\bar{h}l\}$ reflexions centric in (*b*).
Only $\{hki0\}$ reflexions centric in (*c*).
All three principal zones centric in (*d*).
Every zone centric in (*e*).

Some examples of the use of this method and full details of the procedure have already been published (Howells *et al.* 1949, 1950): for example, the confirmation of the choice of $I2$ by Hargreaves & Taylor (1941) for *m*-tolidine dihydrochloride and the space group $P2/a$ for phosphorus triphenyl (Howells, 1949). More recently the space group of nitronium perchlorate, NO_2ClO_4, has been established as Cc by this method (Truter, 1950).

It is concluded from the extended determinative table that the only space groups not resolved by the distribution method are:‡

$$\left.\begin{matrix} I222 \\ I2_12_12_1 \end{matrix}\right\} \quad \left.\begin{matrix} I23 \\ I2_13 \end{matrix}\right\}$$

It is also evident that the usefulness of this method does not end with the assignment of a space group. If we consider $Pnm(2)$, whose new diffraction symbol is

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† A number of cyclostyled copies of this new determinative table have been prepared. The space groups appear in the order and orientations given by Buerger, and are grouped for comparison into sets that were previously inseparable. Copies are available on request.

‡ Two pairs of trigonal space groups, $C3m1$, $C31m$ and $C\bar{3}m1$, $C\bar{3}1m$, were added to these in a preliminary note (Rogers, 1949), but subsequent examination showed that both pairs are separable by noting the orientation with respect to the reciprocal lattice of the planes of symmetry within the intensity array (see footnote ‡, p. 456 of this text).

mmmPn$-=$, it is clearly possible to identify the diad axis unambiguously. This is equally true for *Pmm*(2), where the information is perhaps even more valuable, and would be obtained when distinguishing this space group from *P*222 and *Pmmm*. Many other examples of a similar sort occur, so that reference to the new table of diffraction symbols will frequently assist in the unravelling of structures.

Table 1. *Centric sets of reflexions produced by each symmetry element*

Symmetry axes chosen parallel to [001].

A = acentric; C = centric.

	General reflexions (hkl)		Transverse zone ($hk0$)		Parallel row ($00l$)	
Symmetry elements	Distribution	$n=S/\Sigma$	Distribution	$n=S/\Sigma$	Distribution	$n=S/\Sigma$
1	A	1	A	1	A	1
$\bar{1}$	C	1	C	1	C	1
$2(2_1)$	A	1	C	1	A	2
$\bar{2}(a, b, c, n, d)$	A	1	A	2	C	1
$3(3_{1,2})$	A	1	A	1	A	3
$\bar{3}$	C	1	C	1	C	3
$4(4_{1-3})$	A	1	C	1	A	4
$\bar{4}$	A	1	C	1	C	2
$6(6_{1-5})$	A	1	C	1	A	6
$\bar{6}$	A	1	A	2	C	3

Table 2. *The statistical characteristics of the thirty-two crystal classes*

Crystal class	New diffraction symbol	Centric sets	Operators	Multiples
1	$\bar{1}P$	None	$[C_1]$	1/1
$\bar{1}$	$\bar{1}\underline{P}$	All	$[C_i]$	1/1
m	$2/mP-/-$	$(0k0)$	$[C_h]$	1/2
2	$2/mP-/=$	$(h0l)$	$[C_2]=[C_v]$	2/1
$2/m$	$2/m\underline{P}-/-$	All	$[C_{2h}]=[C_2]\,[C_h]$	2/2
$mm2$	$mmmP--=$	$[(hk0)$ masks $(h00), (0k0)]$	$[C_{2v}]=[C_h]\,[C_v]$; do.; $[C_v]^2$	2/2; 2/2; 4/1
222	$mmmP===$	3 principal zones only	$[D_2]=[C_2]$; $[C_2]$; $[C_2]$	2/1; 2/1; 2/1
mmm	$mmm\underline{P}---$	All	$[D_{2h}]=[C_h]\,[C_v]^2$; do.; do.	4/2; 4/2; 4/2
4	$4/mP-/=$	$(hk0)$	$[C_4]$	4/1
$\bar{4}$	$4/mP\overset{\wedge}{-}/=$	$(hk0)$; $(00l)$	$[S_4]$	2/1
$4/m$	$4/m\underline{P}-/-$	All	$[C_{4h}]=[C_4]\,[C_h]$	4/2
$\bar{4}2m$	$4/mmmP-/==-$	$[(hk0), \{hh0\}]$; $[\{h0l\}, (00l)]$	$[D_{2d}]=[S_4]\,[C_v]$; $[C_2]$; $[C_v]\,[C_h]$	4/1; 2/1; 2/2
$4mm$	$4/mmmP-/=--$	$[(hk0), \{h00\}, \{hh0\}]$	$[C_{4v}]=[C_4]\,[C_v]$; $[C_v]\,[C_h]$; $[C_v]\,[C_h]$	8/1; 2/2; 2/2
42	$4/mmmP-/===$	$(hk0)$; $\{h0l\}$; $\{hhl\}$	$[D_4]=[C_4]$; $[C_2]$; $[C_2]$	4/2; 2/1; 2/1
$4/mmm$	$4/mmm\underline{P}-/---$	All	$[D_{4h}]=[C_4]\,[C_v]\,[C_h]$; $[C_v]^2\,[C_h]$; do.	8/2; 4/2; 4/2
3	$\bar{3}C-$	None	$[C_3]$	3/1
$\bar{3}$	$\bar{3}\underline{C}-$	All	$[C_{3i}]=[C_3]$	3/1
$3m(1)$	$\bar{3}m1C---$	$\{h0\bar{h}0\}$	$[C_{3v}]=[C_3]\,[C_v]$; $[C_h]$; $[C_v]$	6/1; 1/2; 2/1
$32(1)$	$\bar{3}m1C-=-$	$\{h0\bar{h}l\}$	$[D_3]=[C_3]$; $[C_2]$; $[C_1]$	3/1; 2/1; 1/1
$\bar{3}m(1)$	$\bar{3}m1\underline{C}---$	All	$[D_{3d}]=[C_{3i}]\,[C_v]$; $[C_h]\,[C_2]$; $[C_v]$	6/1; 2/2; 2/1
6	$6/mC-/=$	$(hk0)$	$[C_6]$	6/1
$\bar{6}$	$6/mC-/-$	$(00l)$	$[C_{3h}]=[C_3]\,[C_h]$	3/2
$6/m$	$6/m\underline{C}-/-$	All	$[C_{6h}]=[C_6]\,[C_h]$	6/2
$\bar{6}m2$	$6/mmmC-/--=$	$[\{hhl\}, \{hh0\}, (00l)]$	$[D_{3h}]=[C_3]\,[C_h]\,[C_v]$; $[C_h]\,[C_v]$; $[C_2]\,[C_v]$	6/2; 2/2; 4/1
$6mm$	$6/mmmC-/=--$	$[(hk0), \{hh0\}, \{h00\}]$	$[C_{6v}]=[C_6]\,[C_v]$; $[C_h]\,[C_v]$; do.	12/1; 2/2; 2/2
62	$6/mmmC-/===$	$(hk0)$; $(h0l)$; (hhl)	$[D_6]=[C_6]$; $[C_2]$; $[C_2]$	6/1; 2/1; 2/1
$6/mmm$	$6/mmm\underline{C}-/---$	All	$[D_{6h}]=[C_6]\,[C_h]\,[C_v]$; $[C_v]^2\,[C_h]$; do.	12/2; 4/2; 4/2
23	$m3P=-$	$\{hk0\}$	$[T_1]=[C_2]$; $[C_3]$; $[C_1]$	2/1; 3/1; 1/1
$m3$	$m3\underline{P}--$	All	$[T_h]=[C_2]\,[C_h]\,[C_v]$; $[C_3]$; $[C_v]$	4/2; 3/1; 2/1
$\bar{4}3m$	$m3mP=--$	$[\{hk0\}, \{hh0\}]$	$[T_d]=[S_4]\,[C_v]$; $[C_3]\,[C_v]$; $[C_h]\,[C_v]$	4/1; 6/1; 2/2
43	$m3mP=-=$	$\{hk0\}$; $\{hhl\}$	$[O]=[C_4]$; $[C_3]$; $[C_2]$	4/1; 3/1; 2/1
$m3m$	$m3m\underline{P}---$	All	$[O_h]=[C_4]\,[C_v]\,[C_h]$; $[C_3]\,[C_v]\,[C_h]$; $[C_2]\,[C_v]\,[C_h]$	8/2; 6/2; 4/2

3. The method of averages

During an examination of the space groups $C3m1$, $C31m$ and $C\bar{3}m1$, $C\bar{3}1m$, and before recognizing that the members of each pair are separable as explained in the footnote (p. 457), it was observed that the three-dimensional Patterson synthesis exhibits a feature associated with the plane of symmetry, namely, an accumulation of maxima along that normal to the symmetry plane which passes through the origin. This columnar region of high Patterson density, if parallel to [001], for example, implies that the aggregate of the $hk0$ intensities $A_0\left(=\sum\limits_h\sum\limits_k|F_{hk0}|^2\right)$, is notably larger than the sum for any parallel sheet of the reciprocal lattice, $A_l\left(=\sum\limits_h\sum\limits_k|F_{hkl}|^2\right)$. Furthermore, the Patterson projection [001] on the plane of symmetry will have an integrated origin peak twice that for other projections. We may not, however, conclude from this that A_0 is twice that for other zones, since the peak values at the origin of the projections are not necessarily in the ratio 2 : 1, nor has any allowance been made for the number of terms summed for each zone.

A consideration of symmetry axes led in a similar way to the conclusion that analogous results are exhibited by the row of reciprocal-lattice points parallel to the symmetry axis. When a glide occurs the columnar region of high Patterson density (due to the mirror part of the symmetry operation) persists, but is translated laterally by the glide translation (Harker, 1936). (The translation is not due to the systematic absences, but to the fact that the hkl reflexions then consist of two distinct types. This is touched upon in §4, but will be discussed in detail elsewhere.) Similar remarks apply to screw axes and non-primitive cells.

Wilson (1950) has given a precise interpretation to these observations by showing that in the zones or rows predicted above the local *average* intensity is increased by a small integer, the *average-multiple*. The distribution parameter, S, which occurs in both distribution functions (equations (1), (2)) may be considered for three important sets of reflexions: the general reflexions, zones and central rows of the intensity array. In each set S is the local average of the intensities of *those reflexions which are not systematically absent throughout the set*. Thus when deriving S for general reflexions the systematic absences in a zone due to a glide are included, but those due to a non-primitive cell are excluded. Glide or centring absences are omitted when considering a zone, but a row of screw absences is then included.

For general (hkl) reflexions referred to a primitive cell, S has the general value Σ which is defined as $\sum\limits_{j=1}^{N} f_j^2$, the summation including all atoms within the primitive cell. This has been identified with the local average, $\langle I\rangle$, of the absolute intensities of all general reflexions (Wilson, 1942). For a centred lattice the distribution parameter for the reflexions referred to a primitive lattice can be designated S_p $(=\Sigma_p)$ or, when referred to the centred cell, as S_c. The absolute values of the structure amplitudes of a reflexion referred to these alternative cells are related by

$$|F_c|=k|F_p|, \tag{3}$$

where $k=2$ for A-, B-, C- or I-centring and 4 for F-centring. Hence

$$S_c=k^2S_p, \tag{4}$$

and, since

$$\Sigma_c=\sum_{j=1}^{kN} f_j^2=k\Sigma_p, \tag{5}$$

we conclude that

$$S_c=k\Sigma_c, \quad \text{whereas} \quad S_p=\Sigma_p. \tag{6a, b}$$

The modified distribution parameter must be used whenever general reflexions are referred to a non-primitive cell.

If all the atoms in a projection are resolved, S for the zone has the same value, Σ, that applied to the general reflexions. A projection of the cell contents on a plane of symmetry, however, involves superposition in pairs, so that the unit cell of this projection can be considered to contain half the number of scattering centres, but each with doubled scattering power. In like manner a group of n equivalent atoms related by a rotation axis coalesce in the corresponding line projection to give an n-fold reduction in numbers but an n-fold increase in the scattering power compared with general reflexions. Hence for the zone (or row) concerned

$$S=\sum_{j=1}^{N/n}(nf_j)^2=n\Sigma. \tag{7}$$

Thus the average (and not the aggregate) in a zone parallel to a plane of symmetry is twice that of the general reflexions or of other zones. Similarly, the average of a row in the array parallel, for example, to a tetrad axis has an average four times that for the general reflexions. Table 1 summarizes the zones and rows affected and the multiples appropriate to each symmetry operation.

A two-dimensional projection may be centred as a result of:

(1) lattice (end) centring,
(2) a glide,
or (3) both, as [001] in $Cmma$.

The first of these has already been discussed. The second may be treated in two ways:

(a) Retain the primitive three-dimensional cell and its general parameter Σ, so that for the zone affected

$$S_z=k\Sigma, \tag{8}$$

where $k=2$ for a, b, c or n glides.

(b) Refer the projection to its primitive cell. This is equivalent to re-indexing this zone only in terms of a cell which has no three-dimensional counterpart, and whose general parameter is Σ^*. The zone average S^* is then equal to Σ^*. By either approach the factor $1/k$ ($=\frac{1}{2}$ or 1 respectively) represents the fraction of the reflexions which should appear according to the cell and indices chosen.

The combination of a glide and lattice centring may be treated by either of the last two methods. By the first, equation (8) becomes

$$S=k_1k_2\Sigma_c, \tag{9}$$

where $k_1=2$ for *a*, *b*, *c*, *n* or *d*, $k_2=2$ for *A*, *B*, *C* or *I* and 4 for *F* and Σ_c relates to the centred three-dimensional cell. By the second, the problem is reduced to that of a glide in a primitive cell. The glide *d* can occur only in conjunction with *F*, but the combination *Fd* has a multiple 8 (relative to Σ) and not 16, since it is equivalent in another orientation to *Ia* for which the product $k_1k_2=4$; the change in orientation and cells converting this to 8. Alternatively, an examination of the zone will show that the absences produced by *F* and *d* are not distinct, i.e. some reflexions are suppressed by both and only one-eighth should occur in this zone.

There is, therefore, a close correspondence between the effects produced by a plane of symmetry and a glide: that the average intensity of the reflexions which should occur in the zone (which is by definition the parameter *S*) is twice that occurring elsewhere in the intensity array, whether this be reckoned on the basis of a primitive or a centred cell. This is of importance as it permits the zone multiples for the crystal classes in Table 2 to hold irrespective of whether individual space groups within a class incorporate symmetry planes or glides parallel to the zone.

'Centred' one-dimensional projections are treated in the same way as centred two-dimensional projections and give similar results, so that $s=n\Sigma$ covers both screws and rotors. A full list of values of S/Σ ($=n$ or k according to the method of analysis) is given for both screws and glides by Wilson (1950).

It is concluded, therefore, that the ratio S/Σ for a zone or a row is characteristic of the associated translation-free symmetry operation and is independent of the type of cell in which it is found, provided both *S* and Σ relate to the same cell, i.e. either to the primitive or the centred cell. Table 2, column 5, lists the zones and the rows affected on combining symmetry elements to form the thirty-two point groups and denotes in each the multiples for the row and the zone normal thereto, listed in the conventional order. Thus *mm*(2) gives rise to 2/2, 2/2, 4/1:

$$\begin{cases} h00 & n=2 \quad \text{(lies in } h0l\text{)},\\ 0kl & n=2 \quad \text{(zone parallel to } m\text{)},\end{cases}$$

$$\begin{cases} 0k0 & n=2 \quad \text{(lies in } 0kl\text{)},\\ h0l & n=2 \quad \text{(zone parallel to } m\text{)},\end{cases}$$

$$\begin{cases} 00l & n=4,\\ hk0 & n=1.\end{cases}$$

These multiples can be deduced by reference to the equivalent positions in the cell. Especially in the more complex point groups, however, it is easier to use an operator method which may be illustrated by the third entry in the above symbol. A single plane of symmetry parallel to a reciprocal-lattice row gives $n=2$ for the row but $n=1$ for the transverse zone. Denote this by $[C_v]=2/1$. There are two such planes operating simultaneously in this example. Hence

$$[C_v]^2=2/1\,.\,2/1=4/1. \tag{11}$$

Note that the diad axis is an 'implied' symmetry element arising automatically on combining the two perpendicular planes, and for this reason it is frequently omitted from the designation of this point group. All such implied symmetry elements should be omitted from the operator products. These are listed in Table 2, column 4. This interaction of multiples (which gives *n* as high as 12 in some cases) prevents us from indicating symmetry planes and axes by their symbols in Buerger's diffraction symbols.

A zone without glide absences may have $n=1$ or 2, and the multiple is probably best found by comparing the absolute intensities, or *z* values (Howells *et al.* 1950), of a row of reflexions common to this zone and any other for which *n* is known to be unity. The intensities in each zone are measured, corrected and converted to the absolute scale (see Wilson, 1942), in each case on the assumption that $\langle I\rangle=\Sigma$. They will agree if $n=1$, but have the ratio 2:1 throughout if $n=2$, that is, if the zone is parallel to a plane of symmetry. Alternatively, if the experimental conditions can be approximately duplicated for the recording of each zone, the direct averages may be compared more quickly but less reliably.

The multiple for a row may be 1, 2, 3, 4, 6, 8 or 12, and despite the paucity of the reflexions in the row such large factors should be readily, if only approximately, found. The problem will not often arise because rotor multiplicities are often indicated directly by the Laue symmetry, and diad axes are more readily and more satisfactorily indicated by the transverse centric zone. The average of a row is only necessary for distinguishing 4 from $\bar{4}$, for which only the 00*l* reflexions provide distinguishing features as follows:

4(00*l*)	$\bar{4}$(00*l*)
Acentric $n=4$	Centric $n=2$

The distinction is doubtless better ascertained by the method of averages, as it offers a wider margin of discrimination and is less likely to be affected by paucity of reflexions or (as is shown later) by anomalous structural features. These remarks, of course, apply with equal force to any row problems that may arise.

It is evident that the method of averages is particularly valuable for indicating planes of symmetry in either centric or acentric lattices. As a general rule it is preferable to deal with zones rather than rows, but when large multiples are sought in the latter this is not so important. It is concluded that by this method 28 classes are uniquely indicated, the two pairs $1, \bar{1}$ and $3, \bar{3}$ remaining undivided. As an example we can consider the separation of *Pm*, *P*2 and *P*2/*m*:

	Pm	*P*2	*P*2/*m*	
$0k0$	Centric $n=1$	Acentric $n=2$	$n=2$	All centric
$h0l$	Acentric $n=2$	Centric $n=1$	$n=2$	

Pm is quickly identified by its acentric ($h0l$) zone; $0k0$ would be examined only if there were enough reflexions, or for confirmation of a doubtful distribution. The other two may be distinguished by the multiple for the ($h0l$) zone or by the distribution type of some other zone (say $0kl$). The latter is quick, but the former requires a comparison of the ($h0l$) with some other zone. There is no real hardship in either, as at least one other zone will normally be required for the determination of the structure.

Atoms sometimes lie on the symmetry element under consideration, and do not then contribute to this n-fold increase in the average intensity. When known to occupy such positions they may be allowed for in the statistical treatment by regarding them as coincident groups of n scattering units each of power f_k/n with which a new 'general average', Σ', can be calculated which is exactly $1/n$th of that observed for the affected reflexions:

$$S'=\left\{\frac{1}{n}\sum_{j}(nf_j)^2+\sum_{k}f_k^2\right\}=n\left\{\sum_{j}f_j^2+n\sum_{k}(f_k/n)^2\right\}\equiv n\Sigma'. \quad (12)$$

This special value, Σ', is, of course, used only for the affected row or zone.

Conversely, the departure of the experimental value of n from the correct integer may be used to derive an estimate of the number and kind of atoms lying on this particular symmetry element if structural details are neither known nor suggested by the space group and cell contents. Anomalous values of n in a zone can be estimated with some precision by methods discussed earlier. No such precision is likely when dealing with a row, partly because of the poor resolution in the corresponding projection.

It should be noted that atoms in any other special positions (including those on symmetry elements crystallographically equivalent to that under consideration) will not cause departures from the integral values of n, provided that the atoms are sufficiently well resolved in the projections, nor are the conclusions invalidated by the presence of heavy atoms. It seems likely, therefore, that the method of averages can be employed successfully for structures which do not well fulfil the conditions required by the distribution method.

Finally, it should be observed that this method, like the first, permits the identification of symmetry elements for structural purposes as distinct from the assignment to a space group.

4. The 217 diffraction groups and the space groups $I222$, $I2_12_12_1$; $I23$, $I2_13$

The systematic statistical features of the intensity array discussed in the preceding sections offer in most instances alternative means for the unique identification of the crystal class from a study of X-ray intensity data only. The extensive resolution of space groups is incidental to this and is made possible by differentiation within the crystal class on the basis of the systematic absences, a combination of procedures which fails only for the above two pairs of space groups. Since only zones or central rows in the reciprocal lattice can have multiple averages, and zones, rows or the whole intensity array may be centric, it is evident that these systematic features, together with the Laue symmetry and systematic absences, can be considered as elements combined rather after the manner of a point group (see theorem (3), Buerger, 1949). These combinations, which will be termed 'diffraction groups',† describe the known systematic features present in the intensity array resulting from the diffraction of X-rays by the crystal lattice. They are summarized in Table 3, where the order and the cell orientations follow the *International Tables*. The information deducible by intensity statistics is there summarized within brackets which are placed logically between the Laue symbol and that describing the systematic absences, although in practice both the latter are determined prior to the application of the statistical analysis. (Strictly speaking, the Laue symmetry is deducible from the crystal class criteria, but it is more easily recognized and limits the number of classes which the statistical criteria are required to distinguish.) The multiples are indicated as in § 3, but centric rows or zones are here indicated by enclosing the multiple in round brackets. A centric array is indicated by enclosing the entire statistical summary symbol in round brackets instead of the square ones otherwise used. Row multiples are always given because, as was shown in the last section, they may, through coupling of the symmetry elements, have higher multiples than the zones in which they lie. Rows are, however, indicated as centric only when they are not already included in a centric zone.

Viewed in this way, it is evident that the statistical symbol is derived only from the crystal point group and partakes of similar properties. It is for this reason that space groups containing identical symmetry elements differently disposed cannot be distinguished either by statistical methods or by systematic absences. Fortunately, the only examples are the two pairs at present under discussion.

They may be treated as one problem, the cubic pair being a special case of the orthorhombic pair. The three-dimensional Patterson syntheses, drawn in Fig. 1 for

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† This term has been used by Buerger twice (1946, p. 593; 1950, p. 97) as synonymous with his diffraction symbols. It is proposed, however, to reserve the term for the full set of systematic characteristics and their symbolic representation.

a single atom, show that if such an atom is identifiable in a practical problem these space groups may be distinguished. Thus a comparison of any two principal Patterson projections reveals that peak A is at height $z=0$ in $I222$ and $z=\frac{1}{2}$ in $I2_12_12_1$. The reverse is true for peak B. The same conclusions could also be reached from a comparison of the Harker section at $z=0$ (or $\frac{1}{2}$) with the basal projection. This kind of approach is akin to that followed by Buerger in developing his implication theory, and if suitably studied should not require an identifiable heavy atom since every atom will give rise to analogous relations between the Harker peaks. Such studies reveal that the intensities associated with $I2_12_12_1$ are of two distinct types: (*a*) *hkl* all even, and (*b*) only one index even. The reflexions from $I222$ are all congruent with set (*a*) from $I2_12_12_1$. Both types have the same intensity averages and apart from the principal zones both are acentric. The difference is essentially one of 'structure', but will not be discussed in this paper since the systematic features distinguishing the two types are apparently not statistical in character. The only methods known at present for exhibiting the difference are those based on the Patterson projections and sections. Except in Buerger's implication method these will demand a recognizable atom within the structure, but all of them entail a great deal more labour of experiment and computation than the statistical methods.

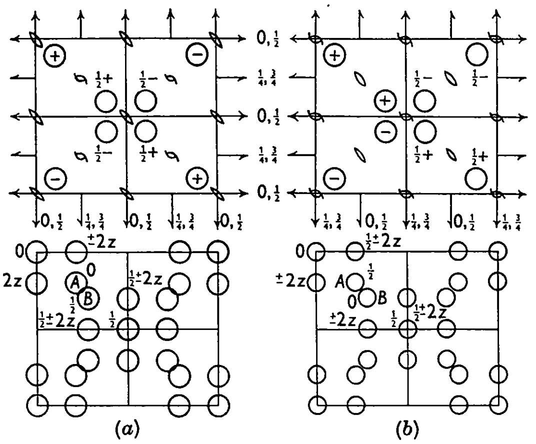

Fig. 1. (*a*) Patterson diagram for $I222$;
(*b*) Patterson diagram for $I2_12_12_1$.

In view of the remarks of the last paragraph and possible future developments it would be unwise to claim that the diffraction group symbols are exhaustive, but the statistical symbols recorded in Table 3 certainly contain all the systematic statistical features discovered so far.

5. Summary

It has been shown that whereas in the past the data directly evident from the diffracted X-ray intensities were insufficient to characterize the crystal class and a majority of space groups, two new statistical procedures provide means for the unique characterization of all crystal classes and make it possible to determine uniquely all but four of the 219 space groups. Some comments have been offered on the choice of statistical method in typical problems and the factors likely to complicate each.

The four refractory space groups $I222$, $I2_12_12_1$ and $I23$, $I2_13$ are not distinguishable by statistical methods but are, at least in principle, separable by the more laborious Patterson methods discussed in §4. It is fortunate that these space groups are rare; Nowacki (1942), in his occurrence statistics, has recorded only two examples of $I23$ and none of the other three. These two were assigned on considerations of molecular symmetry and packing.

The members of each of the eleven pairs of enantiomorphous space groups are also inseparable by statistical methods. The diffraction effects from six pairs are distinguishable by Laue photographs, which do not, however, permit of their identification (ter Berg & Jaeger, 1937).

A symbol (an extension of Buerger's) is introduced to describe the systematic point-group-like features of the intensity array. They represent the 'diffraction groups' of which 217 are recorded in Table 3. The statistical information recorded within them is complete, but the systematic features distinguishing both the enantiomorphous space groups and the remaining four space groups have been omitted.

We may conclude, therefore, that all the 219 space groups are, in principle at least, uniquely determinable from X-ray intensity data only.

Finally, it has been shown that either method can be used to identify symmetry elements for structural purposes, and that in some suitable cases the method of averages can give some indication of the number and nature of the atoms located on individual symmetry elements.

It is a pleasure to acknowledge my indebtedness to Dr A. J. C. Wilson for his generous interest and valuable comments throughout the development of this study; to Prof. Nowacki for assistance in locating substances assigned to several space groups; and to Mrs M. R. Truter for access to data on nitronium perchlorate and permission to mention it here. My thanks are also due to Mr R. Gwynne Howells and Mr D. C. Phillips whose textual criticisms have helped in the removal of a number of obscurities, and to Miss O. Powell for her care in the typing of the tables.

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Table 3. *The 217 diffraction groups*

The multiple gives S/Σ for the principal rows and zones of the intensity array if both S and Σ refer to the same unit cell, whether this be primitive or centred. The sequence and orientations of the space groups conform to the *International Tables.* See text (pp. 460, 461) for description of the nomenclature adopted.

Space group		Diffraction group
C_1^1	$\mathrm{P1}$	$\bar{1}[1/1].P$
C_i^1	$P\bar{1}$	$\bar{1}(1/1).P$
C_s^1	Pm	$2/m[(1)/2].P-/-$
C_s^2	Pc	$.P-/c$
C_s^3	Cm	$.C-/-$
C_s^4	Cc	$.C-/c$
C_2^1	$P2$	$2/m[2/(1)].P-/-$
C_2^2	$P2_1$	$.P2_1/-$
C_2^3	$C2$	$.C-/-$
C_{2h}^1	$P2/m$	$2/m(2/2).P-/-$
C_{2h}^2	$P2_1/m$	$.P2_1/-$
C_{2h}^3	$C2/m$	$.C-/-$
C_{2h}^4	$P2/c$	$.P-/c$
C_{2h}^5	$P2_1/c$	$.P2_1/c$
C_{2h}^6	$C2/c$	$.C-/c$
C_{2v}^1	Pmm	$mmm[2/2;\ 2/2;\ 4/(1)].P---$
C_{2v}^2	Pmc	$.P-c-$
C_{2v}^3	Pcc	$.Pcc-$
C_{2v}^4	Pma	$.P-a-$
C_{2v}^5	Pca	$.Pca-$
C_{2v}^6	Pnc	$.Pnc-$
C_{2v}^7	Pmn	$.P-n-$
C_{2v}^8	Pba	$.Pba-$
C_{2v}^9	Pna	$.Pna-$
C_{2v}^{10}	Pnn	$.Pnn-$
C_{2v}^{11}	Cmm	$.C---$
C_{2v}^{12}	Cmc	$.C-c-$
C_{2v}^{13}	Ccc	$.Ccc-$
C_{2v}^{14}	Amm	$.A---$
C_{2v}^{15}	Abm	$.Ab--$
C_{2v}^{16}	Ama	$.A-a-$
C_{2v}^{17}	Aba	$.Aba-$
C_{2v}^{18}	Fmm	$.F---$
C_{2v}^{19}	Fdd	$.Fdd-$
C_{2v}^{20}	Imm	$.I---$
C_{2v}^{21}	Iba	$.Iba-$
C_{2v}^{22}	Ima	$.I-a-$
D_2^1	$P222$	$mmm[2/(1);\ 2/(1);\ 2/(1)].P---$
D_2^2	$P222_1$	$.P--2_1$
D_2^3	$P2_12_12$	$.P2_12_1-$
D_2^4	$P2_12_12_1$	$.P2_12_12_1$
D_2^5	$C222_1$	$.C--2_1$
D_2^6	$C222$	$.C---$
D_2^7	$F222$	$.F---$
D_2^8	$I222$	$.I---$
D_2^9	$I2_12_12_1$	$.I---$
D_{2h}^1	$Pmmm$	$mmm(4/2;\ 4/2;\ 4/2).P---$
D_{2h}^2	$Pnnn$	$.Pnnn$
D_{2h}^3	$Pccm$	$.Pcc-$
D_{2h}^4	$Pban$	$.Pban$
D_{2h}^5	$Pmma$	$.P--a$
D_{2h}^6	$Pnna$	$.Pnna$
D_{2h}^7	$Pmna$	$mmm(4/2;\ 4/2;\ 4/2).P-na$
D_{2h}^8	$Pcca$	$.Pcca$
D_{2h}^9	$Pbam$	$.Pba-$
D_{2h}^{10}	$Pccn$	$.Pccn$
D_{2h}^{11}	$Pbcm$	$.Pbc-$
D_{2h}^{12}	$Pnnm$	$.Pnn-$
D_{2h}^{13}	$Pmmn$	$.P--n$
D_{2h}^{14}	$Pbcn$	$.Pbcn$
D_{2h}^{15}	$Pbca$	$.Pbca$
D_{2h}^{16}	$Pnma$	$.Pn-a$
D_{2h}^{17}	$Cmcm$	$.C-c-$
D_{2h}^{18}	$Cmca$	$.C-ca$
D_{2h}^{19}	$Cmmm$	$.C---$
D_{2h}^{20}	$Cccm$	$.Ccc-$
D_{2h}^{21}	$Cmma$	$.C--a$
D_{2h}^{22}	$Ccca$	$.Ccca$
D_{2h}^{23}	$Fmmm$	$.F---$
D_{2h}^{24}	$Fddd$	$.Fddd$
D_{2h}^{25}	$Immm$	$.I---$
D_{2h}^{26}	$Ibam$	$.Iba-$
D_{2h}^{27}	$Ibca$	$.Ibca$
D_{2h}^{28}	$Imma$	$.I--a$
S_4^1	$P\bar{4}$	$4/m[(2)/(1)].P-/-$
S_4^2	$I\bar{4}$	$.I-/-$
C_4^1	$P4$	$4/m[4/(1)].P-/-$
C_4^2	$P4_1$	$.P4_1/-$
C_4^3	$P4_2$	$.P4_2/-$
C_4^4	$P4_3$	$.P4_1/-$
C_4^5	$I4$	$.I-/-$
C_4^6	$I4_1$	$.I4_1/-$
C_{4h}^1	$P4/m$	$4/m(4/2).P-/-$
C_{4h}^2	$P4_2/m$	$.P4_2/-$
C_{4h}^3	$P4/n$	$.P-/n$
C_{4h}^4	$P4_2/n$	$.P4_2/n$
C_{4h}^5	$I4/m$	$.I-/-$
C_{4h}^6	$I4_1/a$	$.I4_1/a$
D_{2d}^1	$P\bar{4}2m$	$4/mmm[4/(1);\ 2/(1);\ 2/2].P---$
D_{2d}^2	$P\bar{4}2c$	$.P--c$
D_{2d}^3	$P\bar{4}2_1m$	$.P-2_1-$
D_{2d}^4	$P\bar{4}2_1c$	$.P-2_1c$
D_{2d}^5	$C\bar{4}2m$	$.C-/---$
D_{2d}^6	$C\bar{4}2c$	$.C-/--c$
D_{2d}^7	$C\bar{4}2b$	$.C-/--b$
D_{2d}^8	$C\bar{4}2n$	$.C-/--n$
D_{2d}^9	$F\bar{4}2m$	$.F-/---$
D_{2d}^{10}	$F\bar{4}2c$	$.F-/--c$
D_{2d}^{11}	$I\bar{4}2m$	$.I-/---$
D_{2d}^{12}	$I\bar{4}2d$	$.I-/--d$
C_{4v}^1	$P4mm$	$4/mmm[8/(1);\ 2/2;\ 2/2].P-/---$
C_{4v}^2	$P4bm$	$.P-/-b-$
C_{4v}^3	$P4cm$	$.P-/-c-$
C_{4v}^4	$P4nm$	$.P-/-n-$

Table 3 (*cont.*)

Space group		Diffraction group
C_{4v}^{5}	$P4cc$	$4/mmm[8/(1); 2/2; 2/2].P-/-cc$
C_{4v}^{6}	$P4nc$	$.P-/-nc$
C_{4v}^{7}	$P4mc$	$.P-/--c$
C_{4v}^{8}	$P4bc$	$.P-/-bc$
C_{4v}^{9}	$I4mm$	$.I-/---$
C_{4v}^{10}	$I4cm$	$.I-/-c-$
C_{4v}^{11}	$I4md$	$.I-/--d$
C_{4v}^{12}	$I4cd$	$.I-/-cd$
D_{4}^{1}	$P42$	$4/mmm[4/(1); 2/(1); 2/(1)].P-/---$
D_{4}^{2}	$P42_1$	$.P-/-2_1-$
D_{4}^{3}	$P4_12$	$.P4_1/---$
D_{4}^{4}	$P4_12_1$	$.P4_1/-2_1-$
D_{4}^{5}	$P4_22$	$.P4_2/---$
D_{4}^{6}	$P4_22_1$	$.P4_2/-2_1-$
D_{4}^{7}	$P4_32$	$.P4_1/---$
D_{4}^{8}	$P4_32_1$	$.P4_1/-2_1-$
D_{4}^{9}	$I42$	$.I-/---$
D_{4}^{10}	$I4_12$	$.I4_1/---$
D_{4h}^{1}	$P4/mmm$	$4/mmm(8/2; 4/2; 4/2).P-/---$
D_{4h}^{2}	$P4/mcc$	$.P-/-cc$
D_{4h}^{3}	$P4/nbm$	$.P-/nb-$
D_{4h}^{4}	$P4/nnc$	$.P-/nnc$
D_{4h}^{5}	$P4/mbm$	$.P-/-b-$
D_{4h}^{6}	$P4/mnc$	$.P-/-nc$
D_{4h}^{7}	$P4/nmm$	$.P-/n--$
D_{4h}^{8}	$P4/ncc$	$.P-/ncc$
D_{4h}^{9}	$P4/mmc$	$.P-/--c$
D_{4h}^{10}	$P4/mcm$	$.P-/-c-$
D_{4h}^{11}	$P4/nbc$	$.P-/nbc$
D_{4h}^{12}	$P4/nnm$	$.P-/nn-$
D_{4h}^{13}	$P4/mbc$	$.P-/-bc$
D_{4h}^{14}	$P4/mnm$	$.P-/-n-$
D_{4h}^{15}	$P4/nmc$	$.P-/n-c$
D_{4h}^{16}	$P4/ncm$	$.P-/nc-$
D_{4h}^{17}	$I4/mmm$	$.I-/---$
D_{4h}^{18}	$I4/mcm$	$.I-/-c-$
D_{4h}^{19}	$I4/amd$	$.I-/a-d$
D_{4h}^{20}	$I4/acd$	$.I/acd$
C_{3}^{1}	$C3$	$\bar{3}[3/1].C-$
C_{3}^{2}	$C3_1$	$.C3_1$
C_{3}^{3}	$C3_2$	$.C3_1$
C_{3}^{4}	$R3$	$.R-$
C_{3i}^{1}	$C\bar{3}$	$\bar{3}(3/1).C-$
C_{3i}^{2}	$R\bar{3}$	$.R-$
C_{3v}^{1}	$C3m1$	$\bar{3}m1[6/1; (1)/2; 2/1].C---$
C_{3v}^{2}	$C31m$	$\bar{3}1m[6/1; 2/1; (1)/2].C---$
C_{3v}^{3}	$C3c1$	$\bar{3}m1[6/1; (1)/2; 2/1].C-c-$
C_{3v}^{4}	$C31c$	$\bar{3}1m[6/1; 2/1; (1)/2].C--c$
C_{3v}^{5}	$R3m$	$\bar{3}m1[6/1; (1)/2; 2/1].R---$
C_{3v}^{6}	$R3c$	$\bar{3}m1[6/1; (1)/2; 2/1].R-c-$
D_{3}^{1}	$C312$	$\bar{3}1m[3/1; 1/1; 2/(1)].C---$
D_{3}^{2}	$C321$	$\bar{3}m1[3/1; 2/(1); 1/1].C---$
D_{3}^{3}	$C3_112$	$\bar{3}1m[3/1; 1/1; 2/(1)].C3_1--$
D_{3}^{4}	$C3_121$	$\bar{3}m1[3/1; 2/(1); 1/1].C3_1--$
D_{3}^{5}	$C3_212$	$\bar{3}1m[3/1; 1/1; 2/(1)].C3_1--$
D_{3}^{6}	$C3_221$	$\bar{3}m1[3/1; 2/(1); 1/1].C3_1--$
D_{3}^{7}	$R32$	$\bar{3}m1[3/1; 2/(1); 1/1].R---$
D_{3d}^{1}	$C\bar{3}1m$	$\bar{3}1m(6/1; 2/1; 2/2).C---$
D_{3d}^{2}	$C\bar{3}1c$	$\bar{3}1m(6/1; 2/1; 2/2).C--c$
D_{3d}^{3}	$C\bar{3}m1$	$\bar{3}m1(6/1; 2/2; 2/1).C---$
D_{3d}^{4}	$C\bar{3}c1$	$\bar{3}m1(6/1; 2/2; 2/1).C-c-$
D_{3d}^{5}	$R\bar{3}m$	$\bar{3}m1(6/1; 2/2; 2/1).R---$
D_{3d}^{6}	$R\bar{3}c$	$\bar{3}m1(6/1; 2/2; 2/1).R-c-$

Space group		Diffraction group
C_{3h}^{1}	$C\bar{6}$	$6/m[(3)/2].C-/-$
C_{6}^{1}	$C6$	$6/m[6/(1)].C-/-$
C_{6}^{2}	$C6_1$	$.C6_1/-$
C_{6}^{3}	$C6_5$	$.C6_1/-$
C_{6}^{4}	$C6_2$	$.C6_2/-$
C_{6}^{5}	$C6_4$	$.C6_2/-$
C_{6}^{6}	$C6_3$	$.C6_3/-$
C_{6h}^{1}	$C6/m$	$6/m(6/2).C-/-$
C_{6h}^{2}	$C6_3/m$	$.C6_3/-$
D_{3h}^{1}	$C\bar{6}m2$	$6/mmm[6/2; 2/2; 4/(1)].C-/---$
D_{3h}^{2}	$C\bar{6}c2$	$6/mmm[6/2; 2/2; 4/(1)].C-/-c-$
D_{3h}^{3}	$C\bar{6}2m$	$6/mmm[6/2; 4/(1); 2/2].C-/---$
D_{3h}^{4}	$C\bar{6}2c$	$6/mmm[6/2; 4/(1); 2/2].C-/--c$
C_{6v}^{1}	$C6mm$	$6/mmm[12/(1); 2/2; 2/2].C-/---$
C_{6v}^{2}	$C6cc$	$.C-/-cc$
C_{6v}^{3}	$C6cm$	$.C-/-c-$
C_{6v}^{4}	$C6mc$	$.C-/--c$
D_{6}^{1}	$C62$	$6/mmm[6/(1); 2/(1); 2/(1)].C-/---$
D_{6}^{2}	$C6_12$	$.C6_1/---$
D_{6}^{3}	$C6_52$	$.C6_1/---$
D_{6}^{4}	$C6_22$	$.C6_2/---$
D_{6}^{5}	$C6_42$	$.C6_2/---$
D_{6}^{6}	$C6_32$	$.C6_3/---$
D_{6h}^{1}	$C6/mmm$	$6/mmm(12/2; 4/2; 4/2).C-/---$
D_{6h}^{2}	$C6/mcc$	$.C-/-cc$
D_{6h}^{3}	$C6/mcm$	$.C-/-c-$
D_{6h}^{4}	$C6/mmc$	$.C-/--c$
T^{1}	$P23$	$m3[2/(1); 3/1; 1/1].P---$
T^{2}	$F23$	$.F---$
T^{3}	$I23$	$.I---$
T^{4}	$P2_13$	$.P2_1--$
T^{5}	$I2_13$	$.I---$
T_{h}^{1}	$Pm3$	$m3(4/2; 3/1; 2/1).P---$
T_{h}^{2}	$Pn3$	$.Pn--$
T_{h}^{3}	$Fm3$	$.F---$
T_{h}^{4}	$Fd3$	$.Fd--$
T_{h}^{5}	$Im3$	$.I---$
T_{h}^{6}	$Pa3$	$.Pa--$
T_{h}^{7}	$Ia3$	$.Ia--$
T_{d}^{1}	$P\bar{4}3m$	$m3m[4/(1); 6/1; 2/2].P---$
T_{d}^{2}	$F\bar{4}3m$	$.F---$
T_{d}^{3}	$I\bar{4}3m$	$.I---$
T_{d}^{4}	$P\bar{4}3n$	$.P--n$
T_{d}^{5}	$F\bar{4}3c$	$.F--c$
T_{d}^{6}	$I\bar{4}3d$	$.I--d$
O^{1}	$P43$	$m3m[4/(1); 3/1; 2/(1)].P---$
O^{2}	$P4_23$	$.P4_2--$
O^{3}	$F43$	$.F---$
O^{4}	$F4_13$	$.F4_1--$
O^{5}	$I43$	$.I---$
O^{6}	$P4_33$	$.P4_1--$
O^{7}	$P4_13$	$.P4_1--$
O^{8}	$I4_13$	$.I4_1--$
O_{h}^{1}	$Pm3m$	$m3m(8/2; 6/2; 4/2).P---$
O_{h}^{2}	$Pn3n$	$.Pn-n$
O_{h}^{3}	$Pm3n$	$.P--n$
O_{h}^{4}	$Pn3m$	$.Pn--$
O_{h}^{5}	$Fm3m$	$.F---$
O_{h}^{6}	$Fm3c$	$.F--c$
O_{h}^{7}	$Fd3m$	$.Fd--$
O_{h}^{8}	$Fd3c$	$.Fd-c$
O_{h}^{9}	$Im3m$	$.I---$
O_{h}^{10}	$Ia3d$	$.Ia-d$